

4-Methylindan

824-22-6 | DTXSID7073931

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 |

Model Results

Predicted value: 2.31 days

Global applicability domain: Inside

Local applicability domain index: 7.64e-01

Confidence level: 8.92e-01

Nearest Neighbors from the Training Set

| | | |
|----------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|
| <div>Image not found</div> <div>4-Methylindan</div> <div>Measured: 4.93</div> <div>Predicted: 2.31</div> | <div>Image not found</div> <div>1H-Indene, 2-methyl-</div> <div>Measured: 12.5</div> <div>Predicted: 2.48</div> | <div>Image not found</div> <div>3-Methylindene</div> <div>Measured: 12.5</div> <div>Predicted: 2.76</div> |
| <div>Image not found</div> <div>5-Methylindan</div> <div>Measured: 4.93</div> <div>Predicted: 2.25</div> | <div>Image not found</div> <div>Indene</div> <div>Measured: 12.5</div> <div>Predicted: 7.90</div> | |